Haibo Li

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Current Position

Research Fellow, School of Mathematics and Statistics, The University of Melbourne, Sep. 2023 - now

Academic Experience

Aug. 2021 – Aug. 2023

• **Postdoctoral Researcher**, Institute of Computing Technology, Chinese Academy of Sciences (joint with Computing System Optimization Lab, Huawei Technologies)

Sep. 2015 - Jun. 2021

- **Ph.D. in Computational Mathematics**, Department of Mathematical Sciences, Tsinghua University, China
- Thesis: Joint Bidiagonalization Algorithms for the Computation of Partial GSVDs and Discrete Ill-posed Problems with General-form Regularization

Sep. 2011 - Jun. 2015

• Bachelor in mathematics, Taishan College (talent training project), Shandong University, China

Research Interest

My research interests center around utilizing mathematical modeling and computational techniques to address challenging problems arising from scientific computing, matrix computation and data science. The research areas mainly include:

- Inverse and ill-posed problems
- Numerical linear algebra
- Scientific machine learning

Many other topics are also related to my research, such as numerical optimization, numerical PDEs, and statistical learning. My current research focuses on developing machine learning methods for both forward and inverse problems of PDEs.

Papers (by topics)

Numerical linear algebra:

- **Haibo Li**. The joint bidiagonalization of a matrix pair with inaccurate inner iterations, SIAM Journal on Matrix Analysis and Applications (45), 232–259, 2024.
- Zhongxiao Jia, **Haibo Li**. The joint bidiagonalization method for large GSVD computations in finite precision, SIAM Journal on Matrix Analysis and Applications (44), 382–407, 2023 (Alphabetical order)
- Zhongxiao Jia, **Haibo Li**. *The joint bidiagonalization process with partial reorthogonalization*, Numerical Algorithms (88), 965–992, 2021 (Alphabetical order)
- **Haibo Li**. Generalizing the SVD of a matrix under non-standard inner product and its applications to linear ill-posed problems, 2023, submitted to Applied Mathematics and Computation (In review). https://doi.org/10.48550/arXiv.2312.10403
- Haibo Li, Guangming Tan, Tong Zhao. Backward error analysis of the Lanczos bidiagonalization with reorthogonalization, 2022, submitted to Journal of Computational and Applied Mathematics (Minor revision). https://doi.org/10.48550/arXiv.2210.10297

Computational inverse problems:

• **Haibo Li**. Double precision is not necessary for LSQR for solving discrete linear ill-posed problems, Journal of Scientific Computing, 98:55, 2024.

Papers (by topics) (continued)

- **Haibo Li**. Projected Newton method for large-scale Bayesian linear inverse problems, 2024, submitted to SIAM Journal on Optimization (In review). https://doi.org/10.48550/arXiv.2403.01920
- **Haibo Li**, Jinchao Feng, Fei Lu. *Scalable iterative data-adaptive RKHS regularization*, 2024, submitted to SIAM Journal on Scientific Computing (In review). https://doi.org/10.48550/arXiv.2401.00656
- **Haibo Li**. Subspace projection regularization for large-scale Bayesian linear inverse problems, 2023, submitted to Inverse Problems (In review). https://doi.org/10.48550/arXiv.2310.18618
- Haibo Li. A preconditioned Krylov subspace method for linear inverse problems with general-form Tikhonov regularization, 2023, submitted to SIAM Journal on Scientific Computing (Minor revision). https://doi.org/10.48550/arXiv.2308.06577

Scientific machine learning:

- Tong Zhao, **Haibo Li**, Weile Jia, Guangming Tan. *Query by Self*, manuscript, 2022. https://openreview.net/forum?id=dWhS55KGSKy
- **Haibo Li**, Xingxing Wu, Liping Liu, Guangming Tan, Long Wang, Lin-Wang Wang, Weile Jia. *ALKPU: An Active Learning Method for the DeePMD Model with Kalman Filtering*, manuscript, 2023. https://openreview.net/pdf?id=XtUFeCMZcZ

Scientific computing:

• Yujin Yan, **Haibo Li**, Tong Zhao, Lin-Wang Wang, Lin Shi, Tao Liu, Guangming Tan, Weile Jia, Ninghui Sun. 10-million atoms simulation of first-principle package LS3DF on Sugon supercomputer, Journal of Computer Science and Technology, 2023(Corresponding author)

Presentations and Visits

- Invited talk, Subspace Projection Regularization: preconditioned Golub-Kahan bidiagonalization methods for regularizing linear inverse problems, The 67th Annual Meeting of the Australian Mathematical Society (AustMS 2023), Dec. 2023.
- Invited talk, Active learning strategy for neural network force field with ab-initio accuracy based on Kalman filter, Huawei Technologies, Apr. 19, 2023.
- Invited talk, *A mixed precision variant of LSQR for solving discrete linear ill-posed problems*, Research Center for Mathematics and Interdisciplinary Sciences, Shandong University, Mar. 2023.
- Invited talk, A Kalman filter based optimizer for training the neural network force field with first-principles accuracy, Forum for High Performance Computing and Industrial Material Simulations, CCF HPC China 2022, Dec. 2022.
- Lecture series, Kalman filter for training neural networks, Institute of Semiconductors, Chinese Academy of Sciences, Jun. 28, 2022.
- Invited talk, *The joint bidiagonalization process with reorthogonalization*, Forum for Doctoral Students, Tsinghua University, May 2020.
- Invited talk, *Introduction to iterative algorithms for solving large scale ill-posed problems*, Forum in Mathematics and Interdisciplinary Sciences, Research Center for Mathematics and Interdisciplinary Sciences, Shandong University, Nov. 2019.
- Technical report, *Preconditioned MINRES algorithm: basic theory and implementation*, CAEP Software Center for High Performance Numerical Simulation, Sep. 2019
- Visiting Beijing Institute of Applied Physics and Computational Mathematics, Jul. 2019 Oct. 2019.

Projects and Grants

- Construction and application of micro-scientific computing platform driven by Artificial Intelligence. NSFC No.3192270206. 2023.01-2026.12 (participate at Chinese Academy of Sciences)
- Numerical algorithms for partial SVD and GSVD computations of large scale matrices, NSFC No. 12171273. 2022.01-2025.12 (participate at Tsinghua University)

Projects and Grants (continued)

- High order discontinuous Galerkin methods on point clouds, NSFC No. 11801302. 2019.01-2021.12 (participate at Tsinghua University)
- Krylov iterative solvers for large scale ill-posed problems with standard-form regularization, NSFC No. 11771249. 2018.01-2021.12 (participate at Tsinghua University)

Teaching Experience

- Stochastic Mathematical Methods (for undergraduates), teaching assistant, Tsinghua University. 2015.9-2016.1
- Stochastic Mathematical Methods (for undergraduates), teaching assistant, Tsinghua University. 2016.2-2016.6
- Linear Algebra (for undergraduates), teaching assistant, Tsinghua University. 2016.9-2017.1
- Calculus (for undergraduates), teaching assistant, Tsinghua University. 2017.2-2017.6
- Advanced Numerical Analysis (for postgraduates), teaching assistant, Tsinghua University. 2017.9-2018.1
- Calculus (for undergraduates), teaching assistant, Tsinghua University. 2018.2-2018.6
- Numerical Analysis (for postgraduates), teaching assistant, Tsinghua University. 2018.9-2019.1

Supervision and Co-supervision of students

Co-supervised with Prof. Weile Jia:

Ph.D. candidates •

• Yujin Yan, Chinese Academy of Sciences, 2017 – now, (Co-supervised in 2021–2023)

Master students

• Xingxing Wu, Chinese Academy of Sciences, 2020 – 2023, (Co-supervised in 2022–2023)

Undergraduates

- Weijian Liu, Wuhan University of Technology, 2018 2022 (Co-supervised in 2021–2022 at Chinese Academy of Sciences)
- Qiuchen Sha, Beijing Forestry University, 2018 2022 (Co-supervised in 2021–2022 at Chinese Academy of Sciences)

Skills

Scientific computing

• Numerical Analysis, Matrix computation, Machine learning

Programming

• Advanced: MATLAB, Python, Pytorch, JAX

Basic: C/C++, Linux

Language

• English, Chinese

Others

- Certificate of "The Melbourne Academy Program", by Melbourne Centre for the Study of Higher Education, The University of Melbourne. 2023
- Certificate of "AI Young Talents Training Program Computer Vision Series courses", by Institute for Data Science, Tsinghua University. 2019
- Organizers of the first Student Forum of CSIAM Student Branch, in Tsinghua University. 2018
- Outstanding Graduates of Taishan College, Shandong University. 2015
- Mathematics competition of Chinese College Students, Second prize in Shandong Province, China. 2013
- Contemporary Undergraduate Mathematical Contest in Modeling, First prize in Shandong Province, China. 2013
- Academic Excellence Scholarship of Shandong University. 2012, 2013, 2014

Referees

- Weile Jia, Professor, Institute of Computing Technology, Chinese Academy of Sciences. Email: ji-aweile@ict.ac.cn
- Hailong Guo, Senior Lecturer, School of Mathematics and Statistics, The University of Melbourne. Email: hailong.guo@unimelb.edu.au
- $\bullet \ Fei\ Lu, Associate\ Professor,\ Department\ of\ Mathematics,\ Johns\ Hopkins\ University.\ Email:\ feilu@math.jhu.edu$